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II—Natural Gas Fuel and Dry Air

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National Aeronautics
and Space Administration

Scientific and Technical
Information Branch

Summary

A series of computations has been made to produce the equilibrium temperature and gas composition for natural gas fuel and dry air. The computed tables and figures provide combustion gas property data for pressures from 0.5 to 50 atmospheres and equivalence ratios from 0 to 2.0. Only sample tables and figures are provided in this report. The complete set of tables and figures is provided on four microfiche films supplied with this report.

Introduction

A series of computations was made to determine the equilibrium properties of combustion gas products resulting from the combustion of natural gas fuel and dry air. During combustion research it is important that the properties of combustion gases be readily available and in a form that is convenient and useful to the designer and researcher.

In the past, the combustion gas properties of gas turbine fuels as well as a variety of other hydrocarbon fuels have been computed and reported (refs. 1 to 5). These reports have been used extensively at NASA and throughout industry. The computational schemes that have been developed over the years by Huff, Gordon, Zeleznik, and McBride (refs. 6 to 8) form the basis for these reports and have been used to compute combustion gas properties for a wide spectrum of fuel and oxidant combinations. Often, however, the tables and charts have not been prepared for specific fuels. For example, the data of reference 5 are in a tabular form for hydrogen-carbon (H/C) ratios of 1.7, 2.0, and 2.1 for a range of assigned pressures, temperatures, and fuel-air mixtures. The data in this report also include combustion thermodynamic properties for a range of inlet-air temperatures, but the data herein are plotted to facilitate their use. The resulting figures have proven to be extremely useful in combustion research, and copies of such figures have been prepared for a wide variety of fuels. Because of the numerous requests for these figures as well as the interest in high pressure combustion research (ref. 9), we have decided to prepare a new series of figures and tables and extend the applicable range of the parameters covered. The first report of this series

listed data from combustion of ASTM Jet A and dry air (ref. 10).

This report presents tables and figures for the combustion gas properties of natural gas fuel and dry air for pressures from 0.5 to 50 atmospheres, inlet-air temperatures from 250 to 1150 K, and equivalence ratios from 0 to 2. Only sample tables and figures are provided in this report. The complete set of tables and figures is provided on the four microfiche films supplied with this report.

Procedure

The computations for this report were performed using the NASA Lewis chemical equilibrium computer program documented in reference 8 by Gordon and McBride. The computational method uses a free energy minimization method assuming all gases are ideal and interaction among phases can be neglected. The possible products of reaction are Ar, C (graphite), CH₄, CO, CO₂, H, HO₂, H₂, H₂O(l), H₂O, N H₃, N, NO, NO₂, N₂, O, OH, and O₂. These data, the atomic weights, and physical constants are the same as those used in reference 5.

The computations presented in this report were made for natural gas and dry air. The molecular hydrogen-carbon ratio of 3.9 and lower heat of combustion of $48\,813 \times 10^3$ J/kg used are nominal values obtained from the analysis of several samples of natural gas. The actual weight percent of the (1) various hydrocarbons, (2) N₂, (3) O₂, and (4) CO₂ components of a natural gas that were used in the computations are listed at the beginning of table I(a).

Charts of various useful combustion gas properties were also generated and plotted using computer programs. In the past, these figures had to be generated by crossplotting values from the tables. It was possible to avoid the manual crossplotting of tabular data by having the computer calculate the desired values for a given set of input parameters. For example, the plots in figure 1 are of equilibrium combustion temperature generated over a range of inlet-air temperatures, pressures, and fuel-air ratios. This was done by selecting the final equilibrium combustion temperature, assigning a pressure and fuel-air ratio, and then computing, in an iterative manner, the

required value of inlet-air temperature. These computed values were then stored as a data set and figures were produced by the computer. In regions where the results became highly nonlinear, additional computations were performed in order to present the computed results with the same level of accuracy. A careful examination of these regions shows that the curve fit consists of very short linear segments. In a similar fashion, an appropriate iterative procedure was used to produce the other combustion gas property figures.

Results

The computation procedure was used to produce the tables and the figures that are presented with this report. The major portion of the information is included on the four microfiche films enclosed at the back of this report. Only sample tables and figures are shown and discussed within the report.

Tabular Listing

The computations are listed in tabular form on the microfiche. Table I(a) (designated as table I on the microfiche) is a copy of a typical listing of the combustion gas properties and species. Included in each table are the following:

(1) The case number and description of reactants, the oxidant-fuel weight ratio (O/F), the fuel-air weight ratio (F/A), the percent fuel, and the equivalence ratio, ϕ , which is the ratio of the F/A value to the stoichiometric F/A value, are included. The variation or change in case number has been used to specify a different inlet-air temperature; e.g., case 85 (shown) is 250 K; case 87 is 600 K; case 91 is 1150 K.

(2) Combustion gas properties:

- (a) Equilibrium temperature, T , K and $^{\circ}\text{F}$
- (b) Density, ρ , g/cc
- (c) Molecular weight, M
- (d) Specific heat (at constant pressure), C_p , cal/g-K
- (e) Isentropic exponent, $\gamma(s)$ (as defined in ref. 8)
- (f) Sonic velocity, m/sec

(3) Mole fractions of the various combustion gas species are given when the concentration is equal to or greater than 5 parts per million by volume (ppm).

The listing at the beginning of table I(a) is the input information on the fuel and oxidant. Listed are, from left to right, the fuel and oxidant atomic formulas, the weight fraction of each component, the heats of formation, and the inlet temperature (fuel was introduced at 298 K and air for case 85 is 250 K). This is a typical input listing used by Gordon in reference 5. Table I(a) lists the gas

properties and species concentrations for 1820 different combinations of parametric conditions. The parameters and values used are as follows:

- (1) Combustion pressure, atm: 0.5, 1, 1.5, 2, 3, 4, 6, 10, 15, 20, 30, 40, 50
- (2) Inlet air temperature, K: 250, 400, 600, 800, 1000, 1100, 1150 (case numbers 85 through 91, respectively)
- (3) Equivalence ratio, ϕ : 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.85, 0.9, 0.95, 1.0, 1.05, 1.10, 1.15, 1.2, 1.4, 1.6, 1.8, 2.0

Information contained in table I(a) has been used to generate figures 1, 2, 3, and 6.

Table I(b) (designated as table II on the microfiche) lists the combustion gas properties for different combinations of parametric conditions. These tables were computed by assigning pressure, temperature, and fuel-air ratio and then performing iterative calculations to obtain equilibrium composition and properties. The parameters used are the following:

- (1) Pressure, atm: 0.5 to 50 (in steps as indicated previously)
- (2) Temperature, K: 300 to 2800 in 100 K increments
- (3) Fuel-air ratio (weight): 0.000 to 0.100 in increments of 0.010

Information contained in table I(b) has been used to generate figures 4 and 5.

Additional computations, not listed in table I(a) or I(b), were performed to obtain a more accurate presentation of the nonlinear portions of the curves.

Graphical Presentations

Some typical figures have been included to illustrate the nature of the figures available on the included microfiche. Table II is a listing of the parameter variations and the range of computed gas properties for each of the six figures presented herein. Figure 1 gives computed values showing the effect of varying the inlet-air temperature, fuel-air ratio, and combustion pressure on equilibrium gas temperature. This figure covers pressures from 4 to 50 atmospheres. Figures at lower pressures, 0.5 to 4 atmospheres, are available on the microfiche.

Figure 2 is similar to figure 1 except that the equilibrium temperature is plotted as a function of fuel-air ratio for various values of inlet-air temperature at a single specified level of combustion pressure; in this case, 1 atmosphere.

Figure 3 is similar to figure 2 except that temperature rise values are plotted versus fuel-air ratio for a range of inlet-air temperatures, again at the 1-atmosphere pressure level. Curves at other pressure levels are to be found on the microfiche.

Figure 4 presents the variation in the isentropic exponent γ (ref. 8) as a function of the mixture

temperature for various values of fuel-air ratio at single values of combustion pressure; again, at the 1-atmosphere pressure level. For the purposes of this report, mixture temperature and equilibrium temperature may be used interchangeably.

Figure 5 presents the variation in mixture molecular weight as a function of mixture temperature for various fuel-air ratios at specified levels of combustion pressure.

Figure 6 presents the relationship between the computed equilibrium temperature as a function of the initial temperature for various values of the equivalence ratio (ϕ) at specified pressure levels.

Summary of Results

Advanced computational schemes have been used to produce a series of tables and figures specifically for the combustion properties of natural gas fuel and dry air. Complete tabular listings and graphical representations are provided on the four enclosed microfiche.

Lewis Research Center
National Aeronautics and Space Administration
Cleveland, Ohio, January 31, 1985

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TABLE I.—CONCLUDED.

(b) Assigned temperature, pressure, and fuel-air ratio

CASE= 0		O/F=100.0000		F/A= 0.01000		PERCENT FUEL=		0.9901		PHI= 0.1609	
P, ATM	0.5000	0.5000	0.5000	0.5000	0.5000	0.5000	0.5000	0.5000	0.5000	0.5000	0.5000
P, PSIA	7.3	7.3	7.3	7.3	7.3	7.3	7.3	7.3	7.3	7.3	7.3
T, DEG K	1500.0	1400.0	1300.0	1200.0	1100.0	1000.0	900.0	800.0	700.0	600.0	500.0
T, DEG F	2340.3	2060.3	1880.3	1700.3	1520.3	1340.3	1160.3	980.3	800.3	620.3	440.3
RHO, G/CC	1.1683E-4	1.2518E-4	1.3381E-4	1.4206E-4	1.5032E-4	1.5857E-4	1.6682E-4	1.7507E-4	1.8332E-4	1.9157E-4	2.0000E-4
MOL WT	28.760	28.760	28.761	28.761	28.761	28.761	28.761	28.761	28.761	28.761	28.761
CP, CAL/(G)(K)	0.3024	0.2977	0.2932	0.2888	0.2843	0.2799	0.2754	0.2710	0.2665	0.2621	0.2576
GAMMA (S)	1.2964	1.3023	1.3083	1.3145	1.3211	1.3282	1.3366	1.3464	1.3572	1.3687	1.3800
SUN VEL, M/SEC	749.8	726.0	701.2	675.3	648.2	619.7	589.7	558.0	524.1	487.2	449.8
MOLE FRACTIONS		F/A= 0.01000		F/A= 0.01000		F/A= 0.01000		F/A= 0.01000		F/A= 0.01000	
AR	0.00917	0.00917	0.00917	0.00917	0.00917	0.00917	0.00917	0.00917	0.00917	0.00917	0.00917
CO2	0.01723	0.01723	0.01723	0.01723	0.01723	0.01723	0.01723	0.01723	0.01723	0.01723	0.01723
H2O	0.03264	0.03264	0.03264	0.03264	0.03264	0.03264	0.03264	0.03264	0.03264	0.03264	0.03264
H2	0.00118	0.00071	0.00039	0.00019	0.00008	0.00003	0.00001	0.00000	0.00000	0.00000	0.00000
N2	0.76753	0.76778	0.76794	0.76804	0.76812	0.76819	0.76826	0.76833	0.76840	0.76847	0.76854
OH	0.00005	0.00002	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
O2	0.17219	0.17244	0.17261	0.17271	0.17276	0.17279	0.17280	0.17281	0.17281	0.17281	0.17281
CASE= 0		O/F=100.0000		F/A= 0.01000		PERCENT FUEL=		0.9901		PHI= 0.1609	
P, ATM	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
P, PSIA	14.7	14.7	14.7	14.7	14.7	14.7	14.7	14.7	14.7	14.7	14.7
T, DEG K	2800.0	2700.0	2600.0	2500.0	2400.0	2300.0	2200.0	2100.0	2000.0	1900.0	1800.0
T, DEG F	4990.3	4830.3	4670.3	4510.3	4350.3	4190.3	4030.3	3870.3	3710.3	3550.3	3390.3
RHO, G/CC	1.2279E-4	1.2803E-4	1.3358E-4	1.3936E-4	1.4538E-4	1.5164E-4	1.5814E-4	1.6488E-4	1.7186E-4	1.7908E-4	1.8654E-4
MOL WT	28.212	28.376	28.499	28.588	28.651	28.693	28.720	28.737	28.747	28.752	28.756
CP, CAL/(G)(K)	0.6363	0.5678	0.5074	0.4577	0.4184	0.3882	0.3656	0.3487	0.3361	0.3265	0.3189
GAMMA (S)	1.1717	1.1809	1.1920	1.2045	1.2176	1.2304	1.2433	1.2569	1.2705	1.2843	1.2985
SUN VEL, M/SEC	983.3	966.5	950.9	935.8	920.9	905.6	890.5	875.5	860.5	845.5	830.5
MOLE FRACTIONS		F/A= 0.01000		F/A= 0.01000		F/A= 0.01000		F/A= 0.01000		F/A= 0.01000	
AR	0.00917	0.00917	0.00917	0.00917	0.00917	0.00917	0.00917	0.00917	0.00917	0.00917	0.00917
CO2	0.01723	0.01723	0.01723	0.01723	0.01723	0.01723	0.01723	0.01723	0.01723	0.01723	0.01723
H2O	0.03264	0.03264	0.03264	0.03264	0.03264	0.03264	0.03264	0.03264	0.03264	0.03264	0.03264
H2	0.00118	0.00071	0.00039	0.00019	0.00008	0.00003	0.00001	0.00000	0.00000	0.00000	0.00000
N2	0.76753	0.76778	0.76794	0.76804	0.76812	0.76819	0.76826	0.76833	0.76840	0.76847	0.76854
OH	0.00005	0.00002	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
O2	0.17219	0.17244	0.17261	0.17271	0.17276	0.17279	0.17280	0.17281	0.17281	0.17281	0.17281

TABLE II.—LISTING OF PARAMETER VARIATIONS FOR FIGURES 1 to 6

Figure	Fuel-air ratio (weight)	(Fuel-air ratio) (stoichiometric fuel-air ratio), ϕ	Initial temperature, K	Equilibrium temperature, K	Temperature rise, K, kelvins	Combustion pressure, atm	Mixture temperature, K	γ (s)	Molecular weight
1(a)	0.000-0.080	-----	250-1150	500-2600	-----	0.5-4.0	-----	-----	-----
(b)	.060-0.140	-----	↓	2600-1600	-----	0.5-4.0	-----	-----	-----
(c)	.000-0.080	-----	↓	500-2700	-----	4.0-50.0	-----	-----	-----
(d)	.060-0.140	-----	↓	2700-1600	-----	4.0-50.0	-----	-----	-----
2(a)	0.000-0.095	-----	250-1200	250-2550	-----	0.5	-----	-----	-----
(b)	↓	-----	↓	250-2580	-----	1.0	-----	-----	-----
(c)	↓	-----	↓	250-2600	-----	1.5	-----	-----	-----
(d)	↓	-----	↓	250-2620	-----	2.0	-----	-----	-----
(e)	↓	-----	↓	250-2645	-----	3.0	-----	-----	-----
(f)	↓	-----	↓	250-2655	-----	4.0	-----	-----	-----
(g)	↓	-----	↓	250-2675	-----	6.0	-----	-----	-----
(h)	↓	-----	↓	250-2695	-----	10.0	-----	-----	-----
(i)	↓	-----	↓	250-2710	-----	15.0	-----	-----	-----
(j)	↓	-----	↓	250-2725	-----	20.0	-----	-----	-----
(k)	↓	-----	↓	250-2745	-----	30.0	-----	-----	-----
(l)	↓	-----	↓	250-2755	-----	40.0	-----	-----	-----
(m)	↓	-----	↓	250-2760	-----	50.0	-----	-----	-----
3(a)	0.000-0.095	-----	250-1200	-----	0-1950	0.5	-----	-----	-----
(b)	↓	-----	↓	-----	0-1960	1.0	-----	-----	-----
(c)	↓	-----	↓	-----	0-1970	1.5	-----	-----	-----
(d)	↓	-----	↓	-----	0-1975	2.0	-----	-----	-----
(e)	↓	-----	↓	-----	0-1980	3.0	-----	-----	-----
(f)	↓	-----	↓	-----	0-1985	4.0	-----	-----	-----
(g)	↓	-----	↓	-----	0-1990	6.0	-----	-----	-----
(h)	↓	-----	↓	-----	0-2000	10.0	-----	-----	-----
(i)	↓	-----	↓	-----	0-2005	15.0	-----	-----	-----
(j)	↓	-----	↓	-----	0-2010	20.0	-----	-----	-----
(k)	↓	-----	↓	-----	0-2015	30.0	-----	-----	-----
(l)	↓	-----	↓	-----	0-2020	40.0	-----	-----	-----
(m)	↓	-----	↓	-----	0-2020	50.0	-----	-----	-----
4(a)	0.000-0.06213	-----	-----	-----	-----	0.5	300-2800	1.400-1.133	-----
(b)	↓	-----	-----	-----	-----	1.0	↓	1.400-1.139	-----
(c)	↓	-----	-----	-----	-----	1.5	↓	1.400-1.143	-----
(d)	↓	-----	-----	-----	-----	2.0	↓	1.400-1.146	-----
(e)	↓	-----	-----	-----	-----	3.0	↓	1.400-1.150	-----
(f)	↓	-----	-----	-----	-----	4.0	↓	1.400-1.152	-----
(g)	↓	-----	-----	-----	-----	6.0	↓	1.400-1.157	-----
(h)	↓	-----	-----	-----	-----	10.0	↓	1.400-1.162	-----
(i)	↓	-----	-----	-----	-----	15.0	↓	1.400-1.167	-----
(j)	↓	-----	-----	-----	-----	20.0	↓	1.400-1.170	-----
(k)	↓	-----	-----	-----	-----	30.0	↓	1.400-1.174	-----
(l)	↓	-----	-----	-----	-----	40.0	↓	1.400-1.178	-----
(m)	↓	-----	-----	-----	-----	50.0	↓	1.400-1.180	-----
5(a)	0.000-0.06213	-----	-----	-----	-----	0.5	300-2800	-----	28.97-26.00
(b)	↓	-----	-----	-----	-----	1.0	↓	-----	28.97-26.36
(c)	↓	-----	-----	-----	-----	1.5	↓	-----	28.97-26.53
(d)	↓	-----	-----	-----	-----	2.0	↓	-----	28.97-26.64
(e)	↓	-----	-----	-----	-----	3.0	↓	-----	28.97-26.78
(f)	↓	-----	-----	-----	-----	4.0	↓	-----	28.97-26.87
(g)	↓	-----	-----	-----	-----	6.0	↓	-----	28.97-26.98
(h)	↓	-----	-----	-----	-----	10.0	↓	-----	28.97-27.10
(i)	↓	-----	-----	-----	-----	15.0	↓	-----	28.97-27.18
(j)	↓	-----	-----	-----	-----	20.0	↓	-----	28.97-27.23
(k)	↓	-----	-----	-----	-----	30.0	↓	-----	28.97-27.30
(l)	↓	-----	-----	-----	-----	40.0	↓	-----	28.97-27.35
(m)	↓	-----	-----	-----	-----	50.0	↓	-----	28.97-27.38
6(a)	-----	0.10-1.00	250-1250	540-2545	-----	0.5	-----	-----	-----
(b)	-----	↓	↓	540-2580	-----	1.0	-----	-----	-----
(c)	-----	↓	↓	540-2605	-----	1.5	-----	-----	-----
(d)	-----	↓	↓	540-2620	-----	2.0	-----	-----	-----
(e)	-----	↓	↓	540-2645	-----	3.0	-----	-----	-----
(f)	-----	↓	↓	540-2655	-----	4.0	-----	-----	-----
(g)	-----	↓	↓	540-2680	-----	6.0	-----	-----	-----
(h)	-----	↓	↓	540-2700	-----	10.0	-----	-----	-----
(i)	-----	↓	↓	540-2715	-----	15.0	-----	-----	-----
(j)	-----	↓	↓	540-2730	-----	20.0	-----	-----	-----
(k)	-----	↓	↓	540-2750	-----	30.0	-----	-----	-----
(l)	-----	↓	↓	540-2765	-----	40.0	-----	-----	-----
(m)	-----	↓	↓	540-2775	-----	50.0	-----	-----	-----

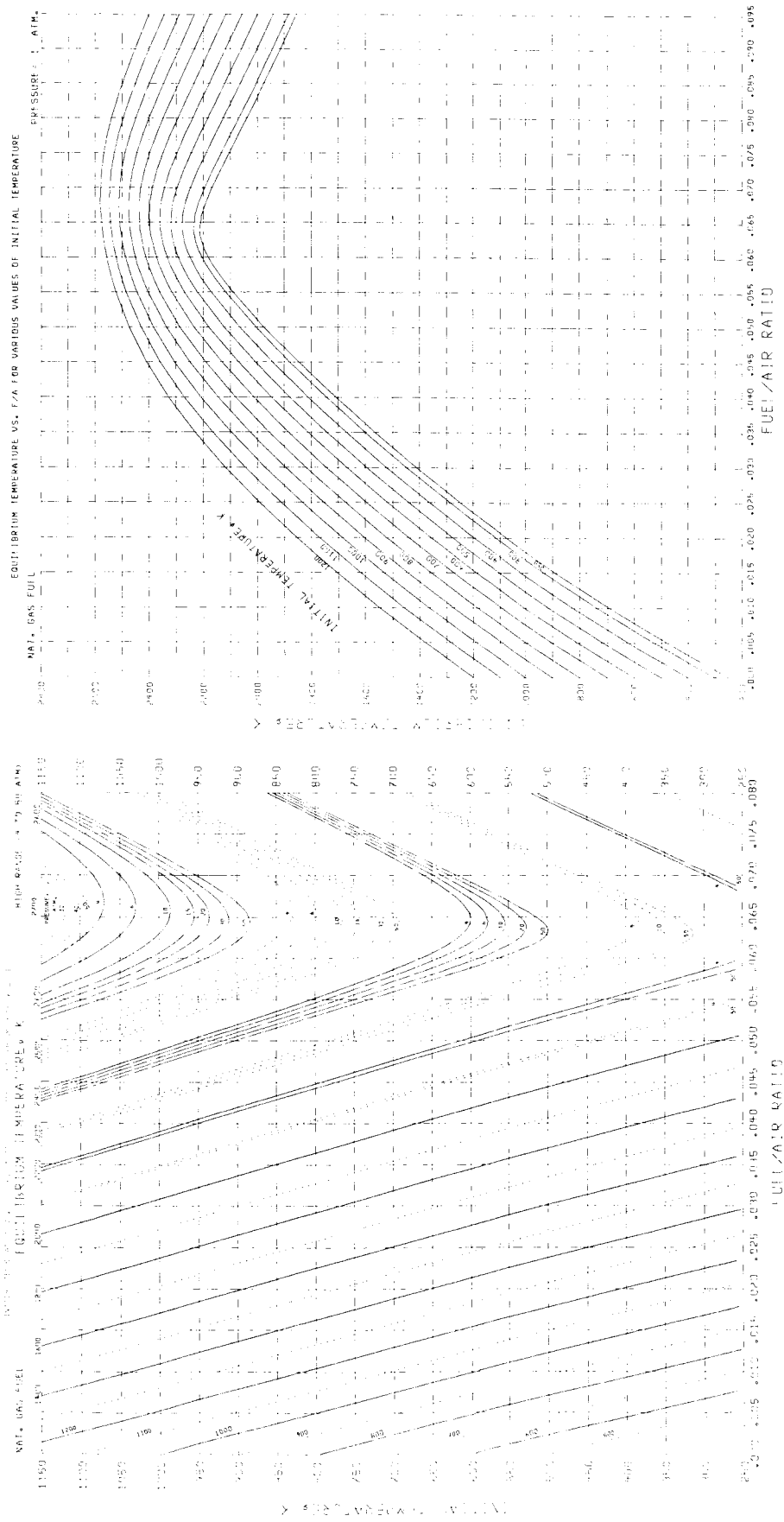


Figure 1.—Equilibrium temperature as function of initial temperature, fuel-air ratio, and pressure range of 4 to 50 atmospheres. Reproduction of microfiche figure 1(c).

Figure 2.—Equilibrium temperature as function of initial temperature and fuel-air ratio at pressure of 1 atmosphere. Reproduction of microfiche figure 2(b).

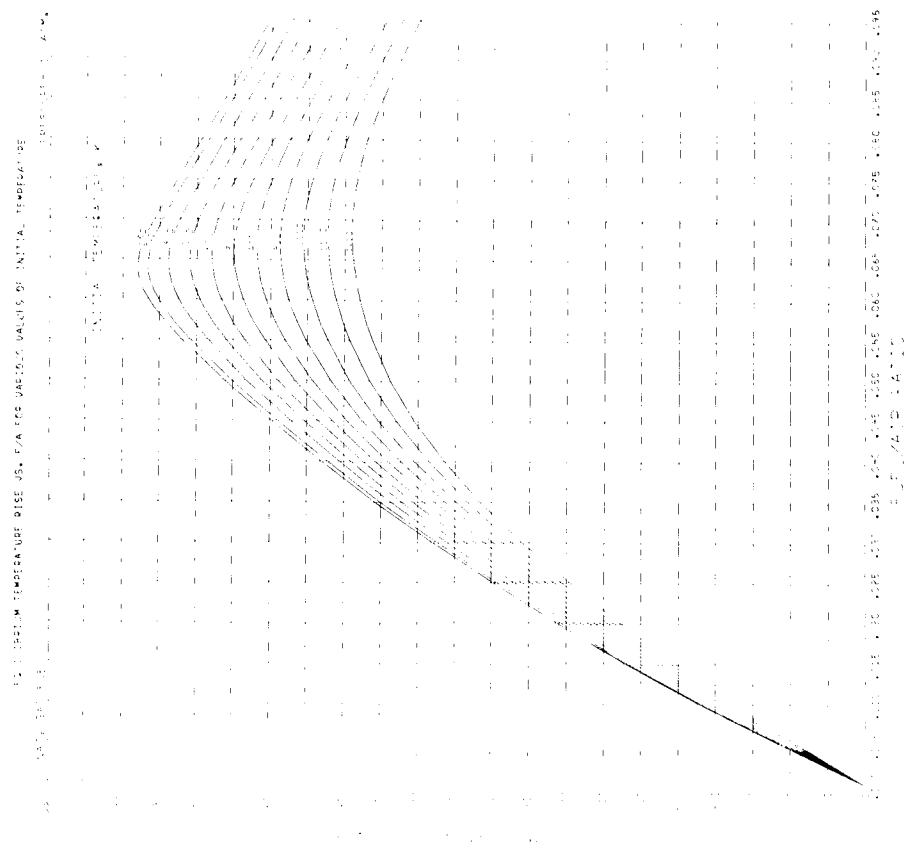


Figure 3.—Equilibrium temperature rise as function of initial temperature and fuel-air ratio at pressure of 1 atmosphere. Reproduction of microfiche figure 3(b).

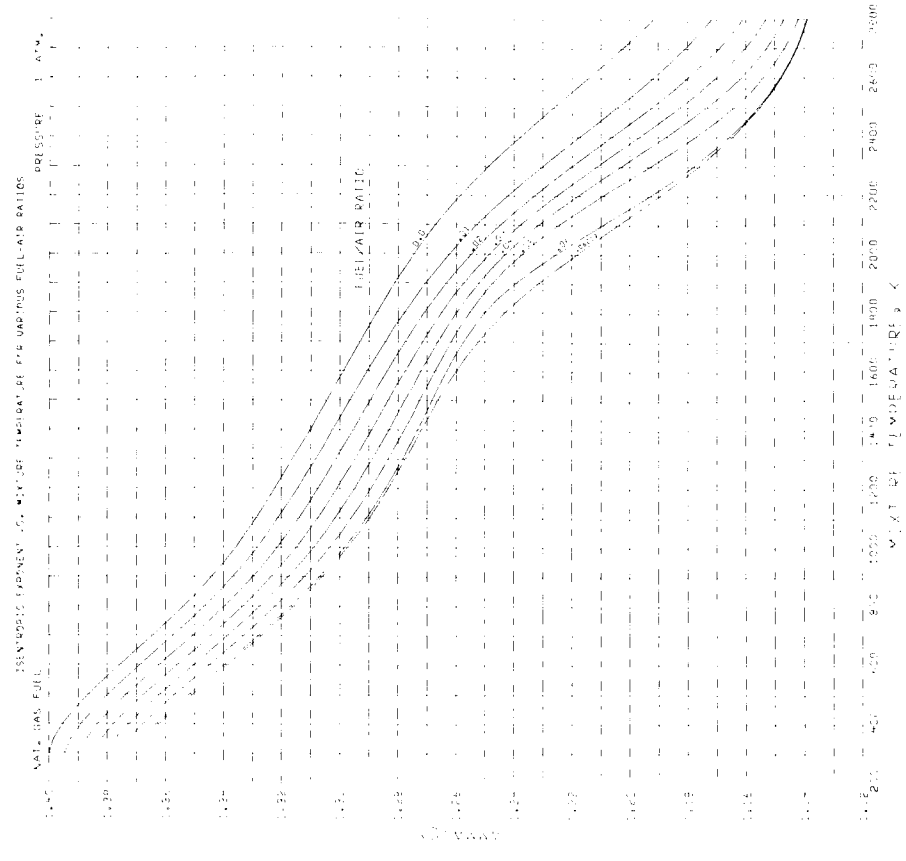


Figure 4.— $\gamma(s)$ as function of mixture temperature and fuel-air ratio at pressure of 1 atmosphere. Reproduction of microfiche figure 4(b).

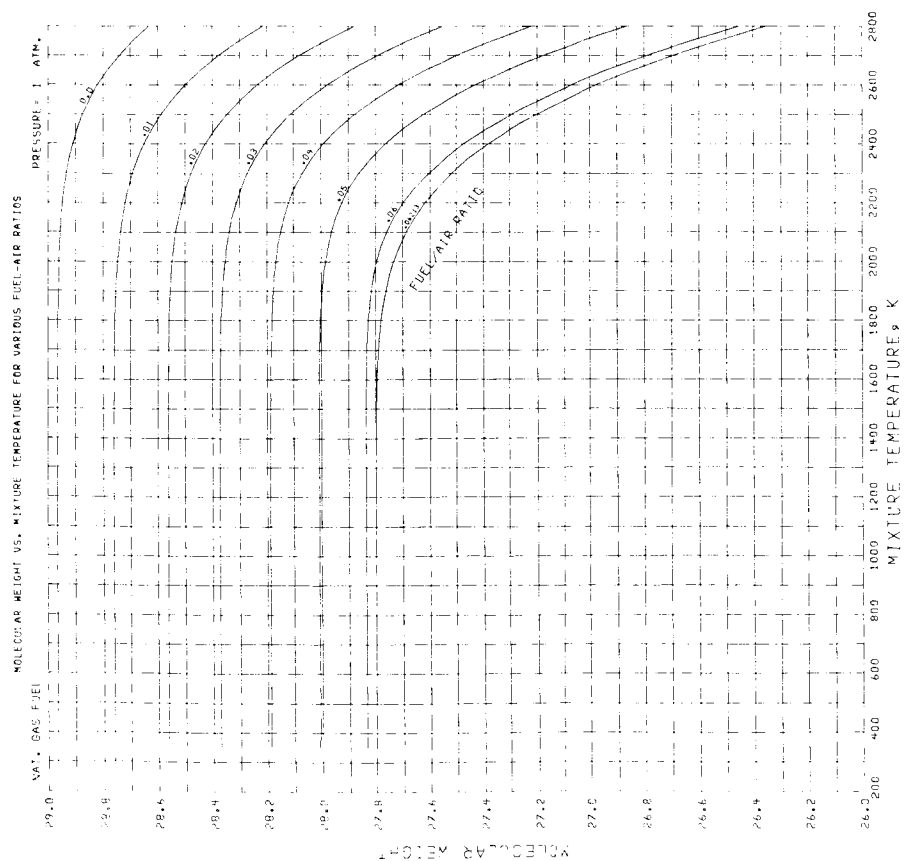


Figure 5.—Molecular weight as function of mixture temperature and fuel-air ratio at pressure of 1 atmosphere. Reproduction of microfiche figure 5(b).

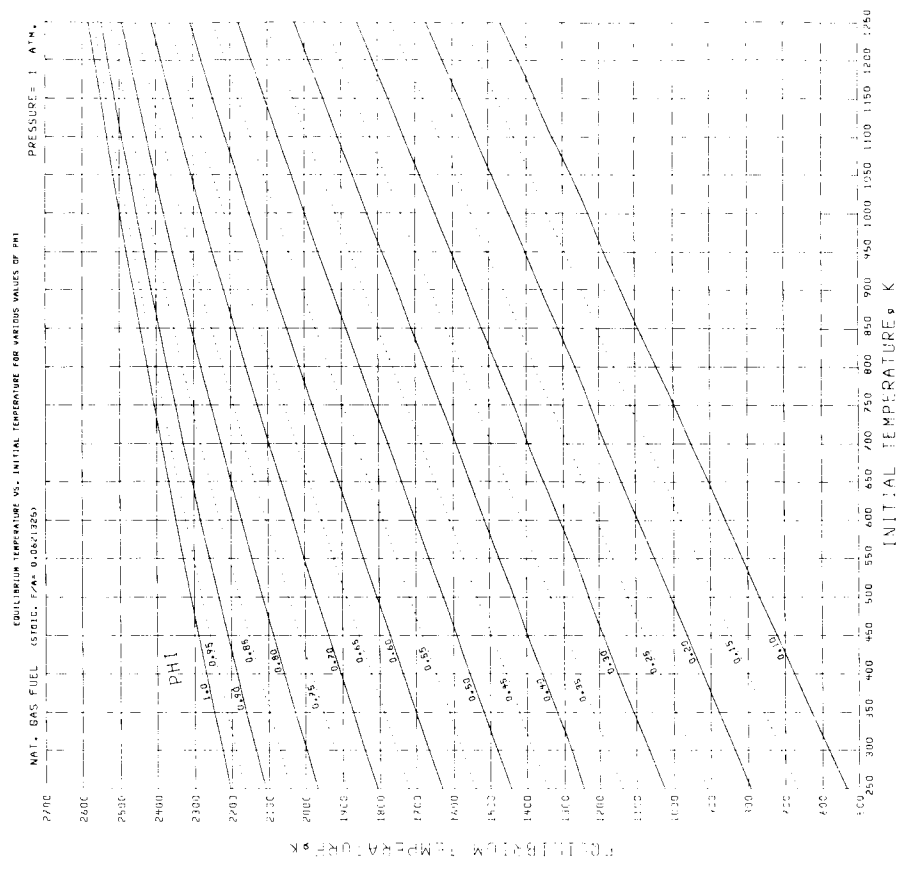


Figure 6.—Equilibrium temperature as function of initial temperature and equivalence ratio φ at pressure of 1 atmosphere. Reproduction of microfiche figure 6(b).

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16. Abstract A series of computations has been made to produce the equilibrium temperature and gas composition for natural gas fuel and dry air. The computed tables and figures provide combustion gas property data for pressures from 0.5 to 50 atmospheres and equivalence ratios from 0 to 2.0. Only sample tables and figures are provided in this report. The complete set of tables and figures is provided on four microfiche films supplied with this report.					
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